



SRNL
SAVANNAH RIVER NATIONAL LABORATORY

techbriefs

StepUp

Engineers at the Savannah River National Laboratory (SRNL) have developed a software toolkit, StepUp, for coarse-node parallelization of chemical process facility simulations. The StepUp toolkit allows a chemical process simulation to be divided across multiple computers on an existing company network. This can be envisioned by treating the computers as separate unit operations or small groupings of unit operations. The material transfers between these unit operation sections become data transmissions over the computer network. In this way, a chemical process facility can be segregated and simulated over a network of computational resources instead of being confined to a single computer.

How Does StepUp Work

The StepUp toolkit is software that coordinates multiple independent chemical process simulations into a single, overall chemical process simulation. By using features such as Visual Basic Automation, the StepUp toolkit directly controls chemical process simulation software such as Aspen Custom Modeler® (ACM). This software control capability is coupled with a message passing protocol to allow remote control of simulation software across a typical office computer network. With this basis, the StepUp toolkit provides an advanced process scheduling system, a centralized data interface, and implements rigorous controls to maintain mass balances and time synchronization between multiple instances of the chemical process software. The StepUp toolkit has taken simulations that were too large to model as a single simulation and divided them into manageable sections that execute over multiple computers.

StepUp Components

StepUp has two executable programs: the local interface and the remote interface. In any StepUp simulation, there is only one instance of the local interface. This interface is launched by the user and provides the overall simulation control. The remote interfaces are launched on the calculation nodes as needed by the local interface. Here local and remote are relative terms used in the context of communications – it is entirely plausible to have a remote interface running on the same computer as the local interface.

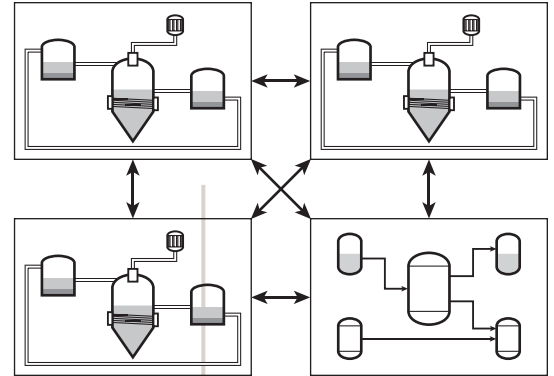
The source code for the two interface programs is written in the Visual Basic 6.0® (VB) programming language. Although the two interfaces are separate programs, the object-oriented character of VB is utilized and there is a subset of code used by both programs; namely, the code defining the communications over the network (PVM Interface) and with the ACM simulation software (ACM Interface) are shared.

at a glance

- increased computational power
- run time flexibility
- greatly simplifies models
- execution time limited only by the slowest model

Benefits of StepUp

There are several benefits realized from employing the StepUp toolkit. They are:



- 1) StepUp significantly simplifies the ACM models.
 - Because each model represents a relatively small, independent section of the system, model development and testing is significantly easier and can be carried out independently from other models.
 - Each model's mathematical solution is not directly coupled with any other model. If one model gets into a difficult solution space and must reduce its step size, it does not slow down the computations in the other models, although it may cause them to wait while it catches up for a material transfer.
 - Individual models can be added, upgraded, or deleted easily and without reworking the overall simulation.
- 2) StepUp improves run time flexibility.
 - The overall simulation can have any number of simultaneous sections.
 - The operator chooses which models to include at run time, allowing for differing simulation size as well as differing levels of computational detail (which is only limited by the capabilities of the underlying models).
- 3) StepUp increases computational power.
 - Instead of sharing a single processor, memory space, and hard disk, each model has its own resources that operate independently.
- 4) StepUp's execution time is limited only by the slowest model.
 - Extra computational detail can be added to other models with no overall cost in execution time.

Technology transfer

SRNL is the applied research and development laboratory at the Savannah River Site (SRS). With its wide spectrum of expertise in areas such as homeland security, hydrogen technology, materials, sensors, and environmental science, SRNL's cutting edge technology delivers high dividends to its customers.

SRNL and SRS are managed for the U.S. Department of Energy by Washington Savannah River Company (WSRC). WSRC is responsible for transferring technologies to the private sector so that these technologies may have the collateral benefit of enhancing U.S. economic competitiveness.

Partnering opportunity

SRNL invites interested companies with proven capabilities in this area of expertise to enter into a licensing agreement with SRNL to market StepUp as a commercial product. Interested companies will be requested to submit a business plan setting forth company qualifications, strategies, activities, and milestones for commercializing StepUp. Qualifications should include past experience at bringing similar products to market, reasonable schedule for product launch, established distribution networks, and evidence of sufficient financial resources for product development and launch.

for more information

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